

Conversion of ^{40}K - ^{87}Rb mixtures into stable molecules

Li-Hua Lu and You-Quan Li

*Zhejiang Institute of Modern Physics and Department of Physics,
Zhejiang University, Hangzhou 310027, P. R. China*

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We study the conversion of ^{40}K and ^{87}Rb atoms into stable molecules through the stimulated Raman adiabatic passage (STIRAP) in photoassociation assisted with Feshbach resonance. Starting with the mean-field Lagrange density, we show that the atom-to-molecule conversion efficiency by STIRAP aided by Feshbach resonance is much larger than that by bare Feshbach resonance. We also study the influence of the population imbalance on the atom-to-molecule conversion.

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I. INTRODUCTION

The study on cold atoms is a remarkable research area which has been extended from monoatomic systems to diatomic systems in recent years [1, 2, 3, 4, 5, 6, 7, 8]. In these experiments, not only degenerate Fermi-Fermi [1, 2, 7] but also Fermi-Bose [3, 4, 5, 6, 8] mixtures are studied. Principally, the degenerate atoms can be converted into molecules through the resonant photoassociation or magnetoassociation (Feshbach resonance). Note that such a compound molecule created by the Feshbach resonance is in a quasibound state and hence energetically unstable. Although the quasibound molecules are energetically unstable, most of fermionic atoms can be efficiently converted into molecules with a long lifetime in experiments [9, 10, 11]. However, as far as we know, the bare Feshbach resonance can not convert either bosonic atoms or Fermi-Bose mixtures into molecules with high efficiency.

To investigate various novel features of cold molecules, one must create ground-state molecules with high atom-to-molecule conversion efficiency. The bare stimulated Raman adiabatic passage (STIRAP) [12, 13] in photoassociation is proposed to enhance the atom-to-molecule conversion efficiency through avoiding quasibound molecules' radiation decay. The success of the STIRAP technique relies on the existence of the coherent population trapping (CPT) state [14], *i.e.*, the system can evolve adiabatically in coherent superposition of stable states. It is easily satisfied for non-interaction systems. However, the inter-particle collisions make it difficult for interaction systems to evolve adiabatically, which limits a practical efficiency of STIRAP. Comparing with the bare STIRAP in photoassociation, the stimulated Raman adiabatic passage aided by magnetoassociation is found to be a more efficient technique whose conversion efficiency is not limited by the collisions between atoms [15, 16, 17]. This technique can be applied to a monoatomic system or a diatomic system. The free atomic states together with the quasibound and ground molecular states constitute a four-level system for which STIRAP aided by magnetoassociation is applicable.

In this paper, we consider systems consisting of fermionic and bosonic atoms and their compounded

fermionic molecules through the technique of STIRAP aided by magnetoassociation. We take the ^{40}K - ^{87}Rb mixture as an example to show that this technique can convert the two species of atoms into molecules with high efficiency. In comparison with STIRAP aided by magnetoassociation, we also show that the bare Feshbach resonance can hardly convert ^{40}K - ^{87}Rb atoms into molecules. The influence of the population imbalance between two species on the atom-to-molecule conversion efficiency is also studied. In the next section, we present our model. In Sec. III we derive the mean-field dynamical equations through the Euler-Lagrange equation then obtain the CPT solutions and the corresponding "two-photon" resonance condition. In Sec. IV we solve the dynamical equations numerically and discuss the corresponding results. Our main conclusions are summarized in Sec. V.

II. THEORETICAL MODEL

We consider a mixture of fermionic and bosonic atoms which are coupled to a quasibound molecular state via Feshbach resonance. Meanwhile, a laser field drives transitions between the quasibound and ground molecular states. For convenience, let $|f\rangle$ and $|b\rangle$ stand for the ground states of fermionic and bosonic atoms in the open channel, and $|m\rangle$ and $|g\rangle$ for the quasibound and ground molecular states in the close channel, respectively. The state $|m\rangle$ is coupled with states $|f\rangle$ and $|b\rangle$ through a magnetic field with coupling strength α' and detuning \mathcal{E}' . Additionally, the states $|m\rangle$ and $|g\rangle$ are coupled with each other through a laser field with the coupling strength Ω' and detuning Δ' . Then the Hamiltonian describing the above system in the interaction picture is written as,

$$\begin{aligned} \hat{H} = & \int d\mathbf{r} \left\{ \sum_i T_i \hat{\Psi}_i^+ \hat{\Psi}_i + \frac{1}{2} \sum_{i,j} \lambda'_{ij} \hat{\Psi}_i^+ \hat{\Psi}_j^+ \hat{\Psi}_j \hat{\Psi}_i \right. \\ & + \frac{\alpha'}{2} [\hat{\Psi}_m^+ \hat{\Psi}_f \hat{\Psi}_b + H.c.] + (\Delta' + \mathcal{E}') \hat{\Psi}_g^+ \hat{\Psi}_g \\ & \left. + \mathcal{E}' \hat{\Psi}_m^+ \hat{\Psi}_m - \frac{\Omega'}{2} [\hat{\Psi}_m^+ \hat{\Psi}_g + H.c.] \right\}, \end{aligned} \quad (1)$$

where $\hat{\Psi}_{i(j)}$ and $\hat{\Psi}_{i(j)}^+$ ($i, j = f, b, m$ and g) are the annihilation and creation field operators. They obey the commutation (+) or anticommutation (-) relations $[\hat{\Psi}_i(\mathbf{r}, t), \hat{\Psi}_j^+(\mathbf{r}', t)]_{\pm} = \delta_{ij}\delta(\mathbf{r} - \mathbf{r}')$ for bosons or fermions, respectively. The coefficient T_i is the kinetic energy due to the particles' motions, and $\lambda'_{ij} = \lambda'_{ji} = 2\pi\hbar^2 a_{ij}/m_{ij}$ the interaction strength between particles with a_{ij} being the s -wave scattering length and $m_{ij} = m_i m_j / (m_i + m_j)$ being the reduced mass. The trapping potential term is not included in the Hamiltonian as we merely consider a uniform system.

The system we considered includes both bosonic and fermionic components. The self-interaction of the bosonic component is distinctly different from that of the fermionic one. The kinetic energy dominates the intra-species interaction for the fermionic component as there is no s -wave scattering for two fermions in the same internal state. This is in marked contrast to the bosonic component for which the interaction energy dominates the kinetic one under most experimental conditions. Thus a very good first approximation is neglecting the intra-species interaction for fermions but neglecting the kinetic energy for bosons. Based on the above consideration, the energy density corresponding to the Hamiltonian Eq. (1), in the Hartree approximation, is given by

$$\begin{aligned} E = & \frac{1}{2} \sum_{i \neq j} \lambda'_{ij} |\psi_i|^2 |\psi_j|^2 + \mathcal{E}' \psi_m^* \psi_m + (\Delta' + \mathcal{E}') \psi_g^* \psi_g \\ & + \frac{\alpha'}{2} [\psi_m^* \psi_f \psi_b + H.c.] - \frac{\Omega'}{2} [\psi_m^* \psi_g + H.c.] \\ & + \frac{1}{2} \lambda'_{bb} |\psi_b|^4 + \sum_{i=\{f, m, g\}} \frac{3}{5} A'_i |\psi_i|^{10/3}, \end{aligned} \quad (2)$$

where ψ_i represents the complex probability amplitude of the i th component and $A'_i = \hbar^2 (6\pi^2)^{2/3} / 2m_i$. The effective self-interaction term $3A'_i |\psi_i|^{10/3} / 5$ related to fermions is called Pauli blocking term. One can find that the effective self-interaction is in different power of $|\psi|$ for bosonic and fermionic components. This will induce distinct difference between the dynamical equation for the bosonic component and that for the fermionic one.

III. MEAN-FIELD DYNAMICS AND CPT STATE

The mean-field approach is an effective method to solve many-body problems (particularly valid for systems with a large number of particles) although the high order quantum correlations are ignored in this approximation [18]. There are different approaches to get the mean-field dynamical equations from Hamiltonian (1). A rigorous approach is expanding bosonic and fermionic field operators in terms of conventional creation and annihilation operators, subsequently, substituting them into the Heisenberg equations of motion for the field operators

(see Ref. [19]). In the mean-field approximation, the evolution of each kind of bosons is determined by a single equation, however, the evolution of N_f fermions is determined by N_f equations. Obviously, it is easy to handle the system with bosons but difficult to handle the system containing a large number of fermions. Another approach is based on the Euler-Lagrange equation with the help of the mean-field Lagrangian density [20, 21]. In this case, the approximation attributes to a single evolution equation for each kind of particles. The difference between the mean-field dynamical equations for bosons and that for fermions arises from the effective self-interaction term.

The method adopted in Refs.[17, 19] is not applicable to our system due to the existence of fermions. We study the system in terms of mean-field Lagrange density,

$$\mathcal{L} = \frac{i}{2} \hbar \sum_i \left(\psi_i^* \frac{\partial \psi_i}{\partial t} - \psi_i \frac{\partial \psi_i^*}{\partial t} \right) - E. \quad (3)$$

Substituting the above mean-field Lagrangian density into the Euler-Lagrange equation $\frac{\partial \mathcal{L}}{\partial \psi_i^*} - \partial_\nu \left(\frac{\partial \mathcal{L}}{\partial (\partial_\nu \psi_i^*)} \right) = 0$, one can get a set of equations for the complex probability amplitudes, ψ_f , ψ_b , ψ_m , and ψ_g . These equations are shown to guarantee the following identities,

$$\begin{aligned} \frac{d}{dt} (|\psi_f|^2 + |\psi_m|^2 + |\psi_g|^2) &= 0, \\ \frac{d}{dt} (|\psi_b|^2 + |\psi_m|^2 + |\psi_g|^2) &= 0, \end{aligned}$$

which means that the total numbers of species f and b are conserved, *i.e.*, $|\psi_f|^2 + |\psi_m|^2 + |\psi_g|^2 = n_f$ and $|\psi_b|^2 + |\psi_m|^2 + |\psi_g|^2 = n_b$ with n_f and n_b being constants. In the following discussion, we assume there is no molecules in the system at the initial time, hence n_f and n_b also denote the initial atom densities of the corresponding species. To simplify the calculation, we let $\phi_i = \psi_i / \sqrt{n_f + n_b}$, then the aforementioned dynamical equations for ψ_i become

$$\begin{aligned} i \frac{\partial \phi_f}{\partial t} &= \sum_{i \neq f} \lambda_{fi} |\phi_i|^2 \phi_f + A_f (\phi_f^* \phi_f)^{2/3} \phi_f + \frac{\alpha}{2} \phi_b^* \phi_m, \\ i \frac{\partial \phi_b}{\partial t} &= \sum_i \lambda_{bi} |\phi_i|^2 \phi_b + \frac{\alpha}{2} \phi_f^* \phi_m, \\ i \frac{\partial \phi_m}{\partial t} &= \sum_{i \neq m} \lambda_{mi} |\phi_i|^2 \phi_m + A_m (\phi_m^* \phi_m)^{2/3} \phi_m + \frac{\alpha}{2} \phi_f \phi_b \\ &\quad - \frac{\Omega}{2} \phi_g + \mathcal{E} \phi_m, \\ i \frac{\partial \phi_g}{\partial t} &= \sum_{i \neq g} \lambda_{gi} |\phi_i|^2 \phi_g + A_g (\phi_g^* \phi_g)^{2/3} \phi_g - \frac{\Omega}{2} \phi_m \\ &\quad + (\Delta + \mathcal{E}) \phi_g, \end{aligned} \quad (4)$$

with the conservation relations $|\phi_f|^2 + |\phi_m|^2 + |\phi_g|^2 = (1 + \delta)/2$ and $|\phi_b|^2 + |\phi_m|^2 + |\phi_g|^2 = (1 - \delta)/2$. Here we introduce $\delta = (n_f - n_b) / (n_f + n_b)$ to characterize the

population imbalance between species f and b , together with further simplified notions: $\lambda_{ij} = \lambda'_{ij}(n_f + n_b)/\hbar$, $\alpha = \alpha'\sqrt{n_f + n_b}/\hbar$, $A_i = A'_i(n_f + n_b)^{2/3}/\hbar$, $\Omega = \Omega'/\hbar$, $\mathcal{E} = \mathcal{E}'/\hbar$, and $\Delta = \Delta'/\hbar$. The population imbalance between two-species atoms is an important parameter affecting the feature of the system. For example, the population imbalance between fermionic atoms for different spin state [22] can induce the superfluid to normal state phase transition.

Unlike the monoatomic system [17], the densities of the fermionic and bosonic atoms may be different, which will affect the conventional two-photon resonance condition. Additionally, the nonlinear terms in our system will be changed because of the Pauli exclusive principle for fermions. We will see that the STIRAP technique aided by Feshbach resonance can convert the two species of atoms into molecules with high efficiency, strictly in contrast to the situation with Feshbach resonance only. We assume that Eqs. (4) support a CPT steady state with $\phi_m = 0$ (the validity of this assumption is supported by our result obtained in the following). We search steady

state solutions of Eqs. (4) with the help of the following trial wave functions,

$$\begin{aligned}\phi_{f,b} &= |\phi_{f,b}| e^{i\theta_{f,b}} e^{-i\mu_{f,b}t}, \\ \phi_{m,g} &= |\phi_{m,g}| e^{i\theta_{m,g}} e^{-i(\mu_f + \mu_b)t},\end{aligned}\quad (5)$$

where μ_f and μ_b are undetermined parameters. Substituting Eqs. (5) into Eqs. (4) and taking $|\phi_m| = 0$, one can find a set of solutions,

$$\begin{aligned}|\phi_f^0|^2 &= \frac{(\alpha^2\delta - \Omega^2) + \sqrt{(\alpha^2\delta - \Omega^2)^2 + 2\alpha^2\Omega^2(1 + \delta)}}{2\alpha^2}, \\ |\phi_b^0|^2 &= |\phi_f^0|^2 - \delta, \quad |\phi_g^0|^2 = \frac{1 + \delta}{2} - |\phi_f^0|^2, \quad \theta_g = \theta_f + \theta_b, \\ \mu_f &= \lambda_{fb}|\phi_b^0|^2 + \lambda_{fg}|\phi_g^0|^2 + A_f|\phi_f^0|^{4/3}, \\ \mu_b &= \lambda_{fb}|\phi_f^0|^2 + \lambda_{bb}|\phi_b^0|^2 + \lambda_{bg}|\phi_g^0|^2,\end{aligned}\quad (6)$$

together with a restriction condition

$$\Delta = -\mathcal{E} + (\lambda_{fb} - \lambda_{fg})|\phi_f^0|^2 + (\lambda_{bb} + \lambda_{fb} - \lambda_{bg})|\phi_b^0|^2 + (\lambda_{fg} + \lambda_{bg})|\phi_g^0|^2 + A_f|\phi_f^0|^{4/3} - A_g|\phi_g^0|^{4/3}. \quad (7)$$

This is a result valid for converting mixtures of fermionic and bosonic atoms into fermionic molecules. The parameters λ_{ij} and A_i can be obtained directly for concrete systems.

IV. NUMERICAL RESULTS FOR CONCRETE SYSTEMS

Now we are in the position to consider a concrete system consisting of two-species atoms (saying ^{40}K and ^{87}Rb) and their compounded fermionic molecules. In order to carry out the numerical calculations, it is necessary to fix magnitudes of the parameters that affect the atom-to-molecule conversion efficiency. As we know, $\mathcal{E}' \approx (2\mu_e + \mu_N)(B - B_m)$ where μ_e and μ_N refer to the electron and nucleus magnetic moments, B the magnetic field (the resonances occur at $B = B_m$) [23]. To evaluate the parameter α' , let us recall the form of the s -wave scattering length between species f and b : $a_{fb} = a(1 - \Delta_{\text{Fes}}/(B - B_m))$. Here a is the scattering length far off resonance and $\Delta_{\text{Fes}} = \alpha'^2 m_{fb} / (2\pi\hbar^2 a(2\mu_e + \mu_N))$ the resonance width with $m_{fb} = m_f m_b / (m_f + m_b)$ being the reduced mass of species f and b . The scattering length a for the ^{40}K - ^{87}Rb mixture determined through Feshbach spectroscopy is about $-185a_0$ with a_0 being the Bohr radius [24], and the expectation value for the width Δ_{Fes} is about -3G [25]. Thus we obtain $\alpha' \approx 9.07 \times 10^{-39}\text{J}$.

To optimize the conversion efficiency in experiment, one can change the detuning \mathcal{E}' and the interaction between species f and b by varying the magnetic field B . Alternatively, one can also fix the magnetic field but vary Ω' to improve the conversion efficiency. In our numerical calculation, the magnetic field B is fixed to simplify the experimental procedure. For $B = 546.4\text{G}$, the corresponding s -wave scattering length between species f and b is about $2950a_0$. If the total atomic density $n_f + n_b$ is about 10^{20}m^{-3} and the s -wave scattering length between ^{87}Rb atoms is about $100a_0$, it is easy to obtain $\lambda_{fb} = 0.23\alpha$, $\lambda_{bb} = 0.0056\alpha$, $A_f = 0.3\alpha$, $A_m = A_g = 0.09\alpha$ and $\mathcal{E} = -4.1\alpha$. Since there are no good estimations on molecular scattering lengths, we take the interaction strengths involving molecules to be zero. The full set of Eqs. (4) are solved numerically by choosing a time-dependent Rabi frequency adopted in Ref. [17]

$$\Omega(t) = \Omega_{\text{max}} \left[1 - \tanh\left(\frac{t - t_0}{\tau}\right) \right], \quad (8)$$

and Δ given by Eq. (7). Here Ω_{max} , t_0 and τ are constants to be determined by the laser coupling of the two molecular states. We take $\Omega_{\text{max}} = 200\alpha$, $t_0 = 120/\alpha$, $\tau = 40/\alpha$ and assume that there exist no molecules in the system at the initial time, *i.e.*, $\phi_{m,g} = 0$ at $t = 0$. Such an assumption can be realized in experiment through the following procedure. At the initial time, fix the magnetic field at the value far off resonance

and prepare ^{40}K and ^{87}Rb atoms in their ground states $|f\rangle = |F = 9/2, m_F = -9/2\rangle$ and $|b\rangle = |1, 1\rangle$, respectively. Turn on the laser pulse and fix its amplitude at Ω_{max} , and then let the magnetic field be suddenly close to the Feshbach resonance point. Some numerical results on atom-to-molecule conversion with $B = 546.4\text{G}$ are plotted in Fig. 1. Figure 1(a) exhibits that $|\phi_m|^2 \sim 0$ at the initial time, which implies the populations fulfil the CPT solutions while a small deviation begins to appear at about $t = 300/\alpha$. In spite of the small deviation, the final conversion efficiency $2|\phi_g(t = \infty)|^2$ is about 60%. Note that the Feshbach resonance can not convert ^{40}K - ^{87}Rb atoms into molecules with such a high efficiency. We plot the conversion efficiency as a function of δ in Fig. 1(b). Clearly, there is a significant influence of δ on the conversion efficiency.

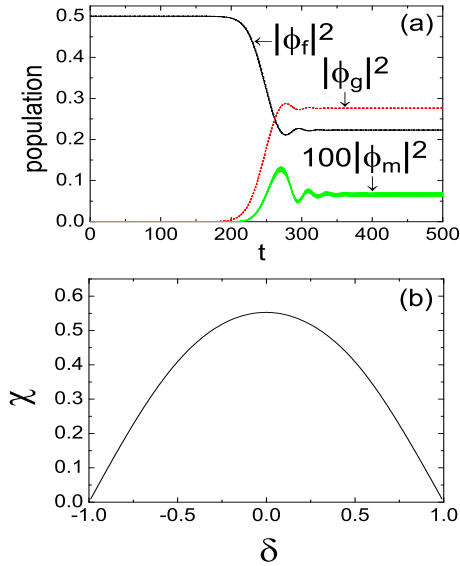


FIG. 1: (color online) Panel (a) shows the time dependence of the population of particles for $\delta = 0$. Panel (b) is the conversion efficiency $\chi = 2|\phi_g(t = \infty)|^2$ as the function of the population imbalance δ . The parameters are $\lambda_{fb} = 0.23$, $\lambda_{bb} = 0.0056$, $\lambda_{fm} = \lambda_{fg} = \lambda_{bm} = \lambda_{bg} = \lambda_{mg} = 0$, $A_f = 0.3$, $A_m = A_g = 0.09$ and $\mathcal{E} = -4.1$. Time is in unit of $1/\alpha$ and all other coefficients are in units of α .

As we know, except λ_{fb} and \mathcal{E} , the other parameters do not change with respect to the magnetic field. Thus the magnetic field affects the conversion efficiency through the detuning \mathcal{E} and the interaction between species f and b . To show the influence of the magnetic field B , we plot the atom-to-molecule conversion efficiency versus the magnetic field in Fig. 2. One can see that the strength of magnetic field can affect the conversion efficiency distinctly and the curves are not continuous at $B = 546.6\text{G}$. Such a discontinuity is brought in by the divergence of the interaction λ_{fb} at $B = 546.6\text{G}$.

In comparison to the STIRAP aided by Feshbach resonance technique, the results for the bare Feshbach resonance are plotted in Fig. 3. The results are obtained by

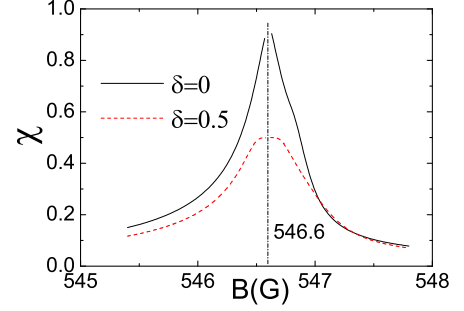


FIG. 2: (color online) The atom-to-molecule conversion efficiencies $2|\psi_g(t = \infty)|^2$ versus the magnetic field B for different population imbalance δ . The parameters except λ_{fb} and \mathcal{E} are the same as that in Fig. 1 (a).

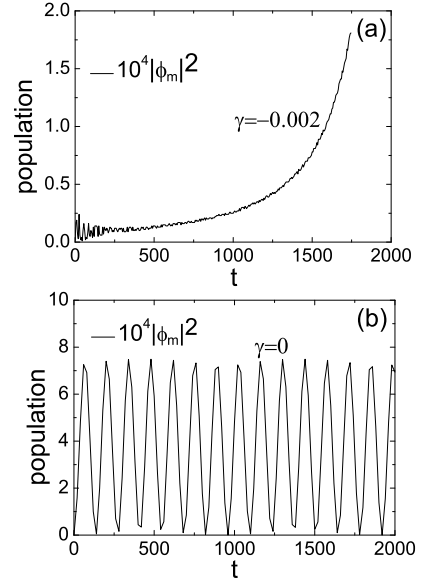


FIG. 3: (color online) The time dependence of molecular population for the Feshbach resonance. The parameters are $\delta = 0$, $\lambda_{fb} = 0.23$, $\lambda_{bb} = 0.0056$, $\lambda_{fm} = \lambda_{bm} = 0$, $A_f = 0.3$, $A_m = 0.09$ and $\mathcal{E} = -4.1$. Time is in unit of $1/\alpha$ and all other coefficients are in units of α .

solving the following set of equations:

$$\begin{aligned}
i\frac{\partial\phi_f}{\partial t} &= \sum_{i=\{b,m\}} \lambda_{fi}|\phi_i|^2\phi_f + A_f(\phi_f^*\phi_f)^{2/3}\phi_f + \frac{\alpha}{2}\phi_b^*\phi_m, \\
i\frac{\partial\phi_b}{\partial t} &= \sum_{i=\{f,b,m\}} \lambda_{bi}|\phi_i|^2\phi_b + \frac{\alpha}{2}\phi_f^*\phi_m, \\
i\frac{\partial\phi_m}{\partial t} &= \sum_{i=\{f,b\}} \lambda_{mi}|\phi_i|^2\phi_m + A_m(\phi_m^*\phi_m)^{2/3}\phi_m \\
&\quad + \frac{\alpha}{2}\phi_f\phi_b + \mathcal{E}\phi_m.
\end{aligned} \tag{9}$$

Unlike the STIRAP technique, the magnetic field is swept according to $B = B_{\text{ini}} + \gamma t$ (here B_{ini} denotes the initial value of the magnetic field) in the Feshbach resonance approach. The interaction λ_{fb} and the detuning \mathcal{E} therefore change with time in the calculation procedure if $\gamma \neq 0$. From Fig. 3, we find that the Feshbach resonance technique can hardly convert ^{40}K - ^{87}Rb atoms into molecules even if the magnetic field is swept slowly. The magnetic field is brought from the initial value 551G to the final value 547.5G in 2ms in panel (a), whereas the magnetic field is fixed in panel (b) due to $\gamma = 0$.

V. SUMMARY

We studied the atom-to-molecule conversion efficiency for Fermi-Bose mixtures. We took the system consisting of ^{40}K - ^{87}Rb atoms and their compounded molecules as an example to have shown that the STIRAP aided by Feshbach resonance is an efficient scheme for one to convert Fermi-Bose atoms into fermionic molecules. Such a scheme is easy to handle in experiments because it is no more necessary to sweep the magnetic field across the Feshbach resonance. In contrast to the STIRAP aided by Feshbach resonance technique, the bare Feshbach resonance can hardly convert Fermi-Bose atoms into molecules. We showed that the population imbalance δ between two-species atoms is a conserved quantity which is an important parameter affecting the feature of system. We discussed the influence of δ on the atom-to-molecule conversion in the system that consists of Fermi-Bose atoms and their compounded molecules.

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